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ME469: Nalu Overview

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Lecture Objectives

- Nalu Technology Origination: ASC
- Beyond the 32-bit Limit
- Supported Physics
- Supported Numerics
- Low- and High-order
- Moving Mesh (Sliding and Overset)
- Multiphysics
 - Fluid Structure Interaction
 - Conjugate Heat Transfer (CHT)
 - Participating Media Radiation
 - Examples



Core Technology Provided to Nalu Origination: Advanced Simulation and Computing Sierra/Fuego

- Use-case characterized by a highly sooting, turbulent, reacting flow with Participating Media Radiation (PMR), Conjugate Heat Transfer (CHT), and propellant multi-physics coupling

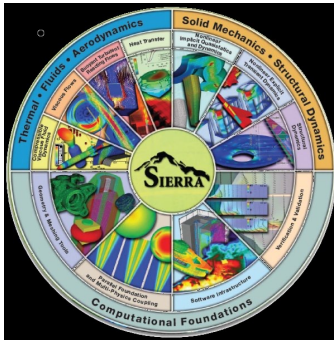


- Complex geometry has driven a generalized, hybrid unstructured discretization approach supporting Hex8, Tet4, Wedge6, and Pyramid5 elements in addition to promotion of Hex8 to Hex27, and Tet4 to Tet10



Goal: Beyond 32-bit Computing

- Circa 2013, many scientific production codes were limited to 32-bit
- Therefore, maximum simulation size for entities, e.g., node, edge, face, element, etc., was ~2.2 billion
- Next Generation Platforms were advocated to overcome poor MPI scaling and power needs to support Exascale computing (10^{18} floating point operations/second)
 - Platform architectures, at that point, were not yet known (still evolving)



+ Advanced Simulation and
Computing Investments



Sierra Toolkit/Trilinos (open-source)

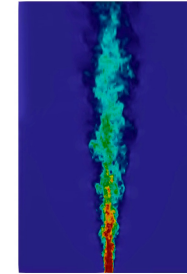
MPI+X parallelism

Support for new architectures



Developed Open-Source BSD-clause 3 Distribution Policy

- Philosophy: Open-source collaborations

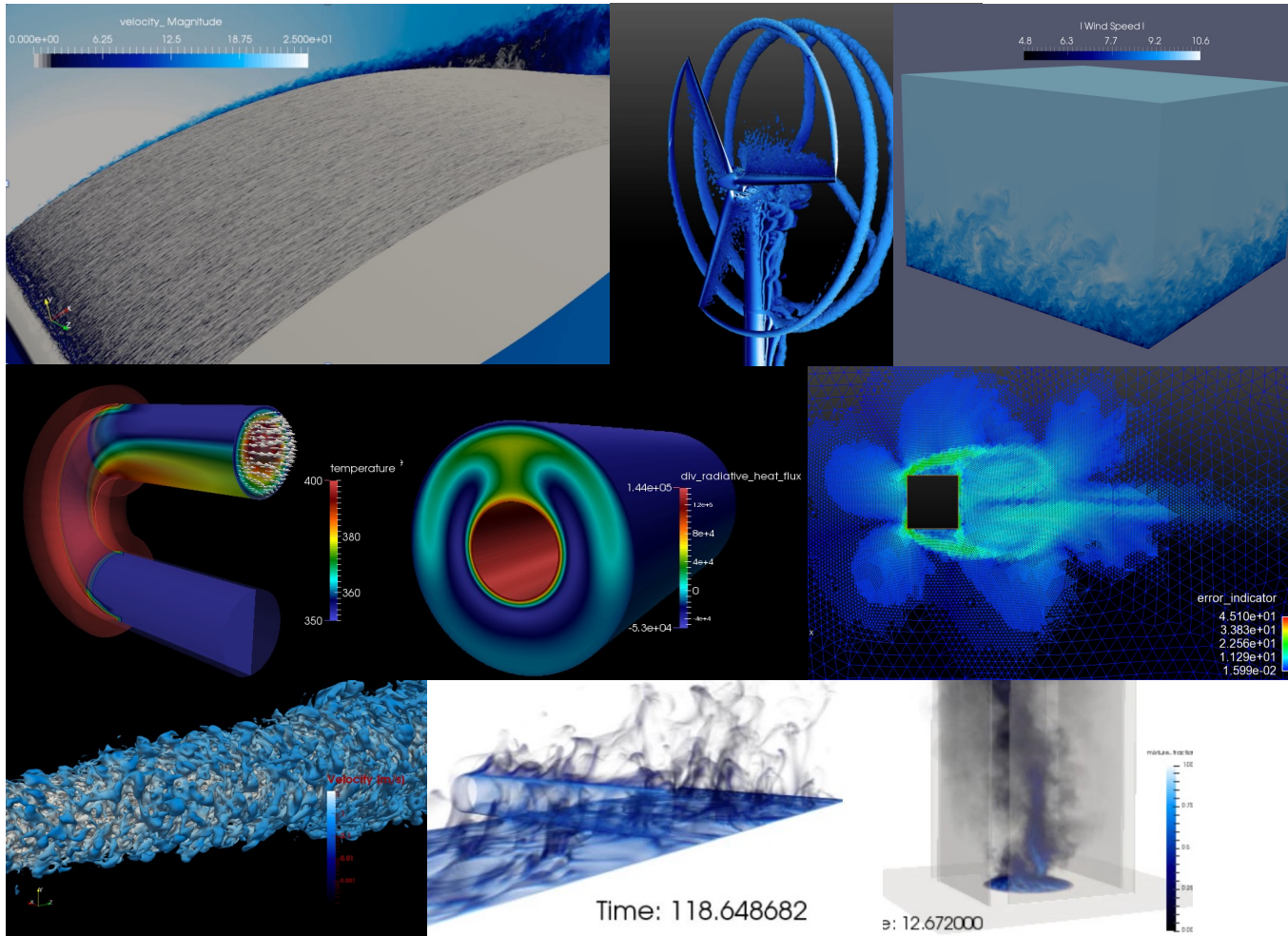


<https://github.com/NaluCFD>





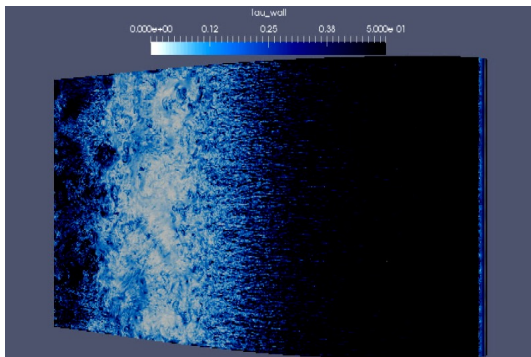
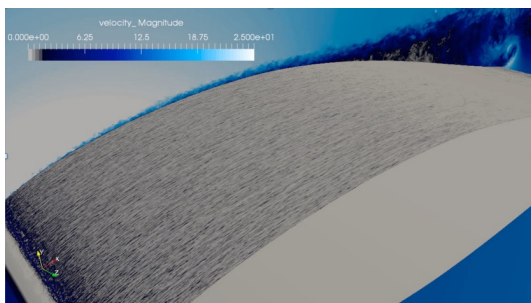
Supported Physics: DNS and LES (even RANS)



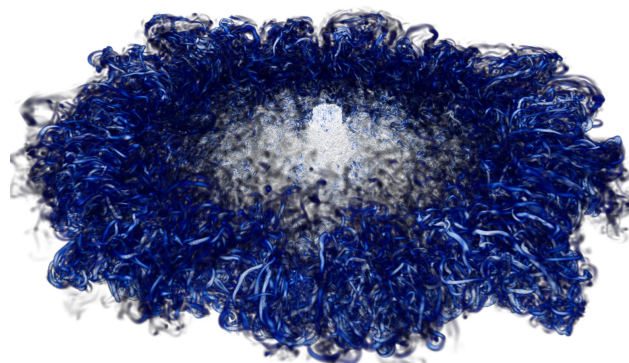


A Note on High Performance Computing

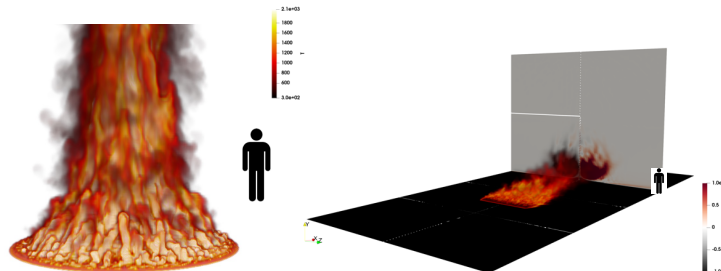
Sandia (and Stanford) are committed to High Performance Computing (HPC) to support is science and engineering objectives: Exercised herein



O(6) billion wind energy application



O(2) billion DNS impinging jet

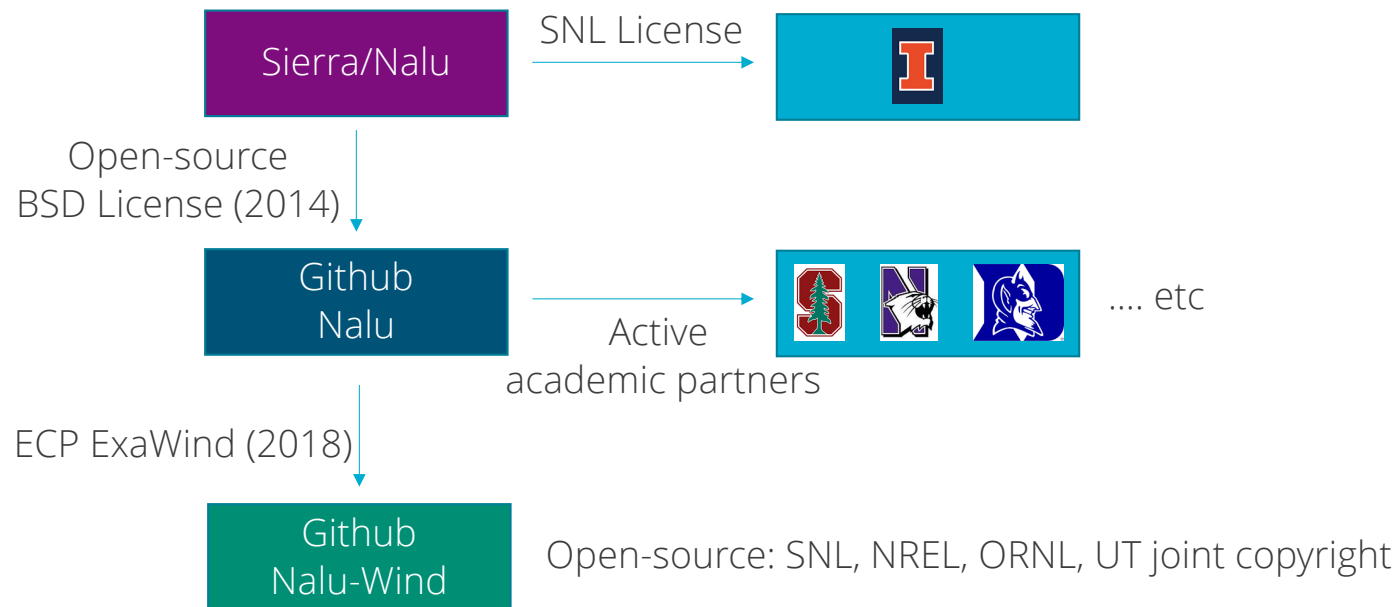


O(200) million multi-physics fire



Nalu Timeline/History

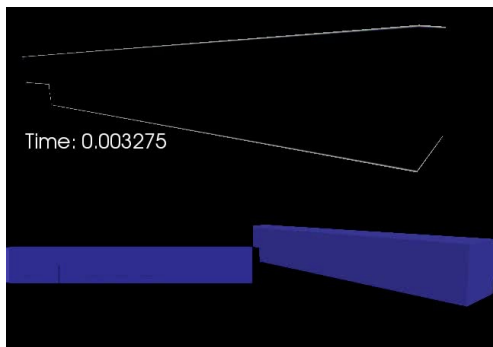
- By CFD standards, this is a relatively new code base



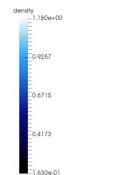


Several Multi-physics Flow Examples From Nalu

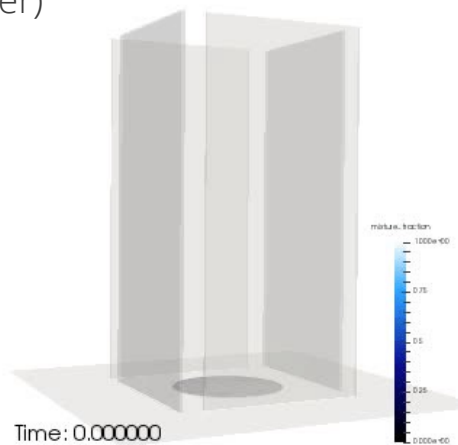
Helium plume (low-/high-order)
R1, 20cm



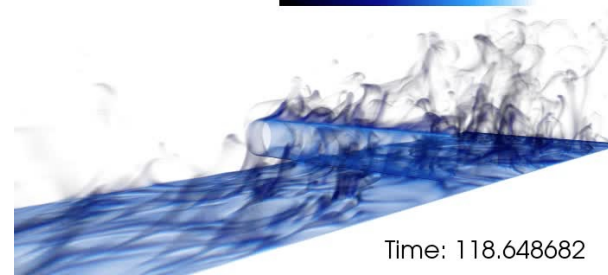
Heated backstep



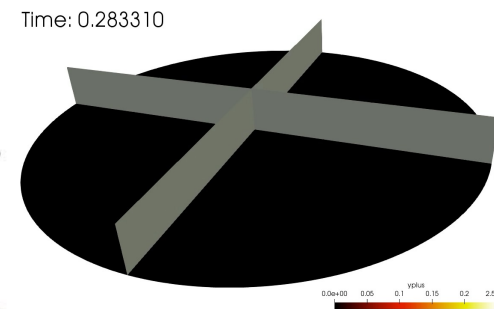
R1, 20cm



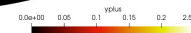
Whirling behavior



Cylinder in cross flow

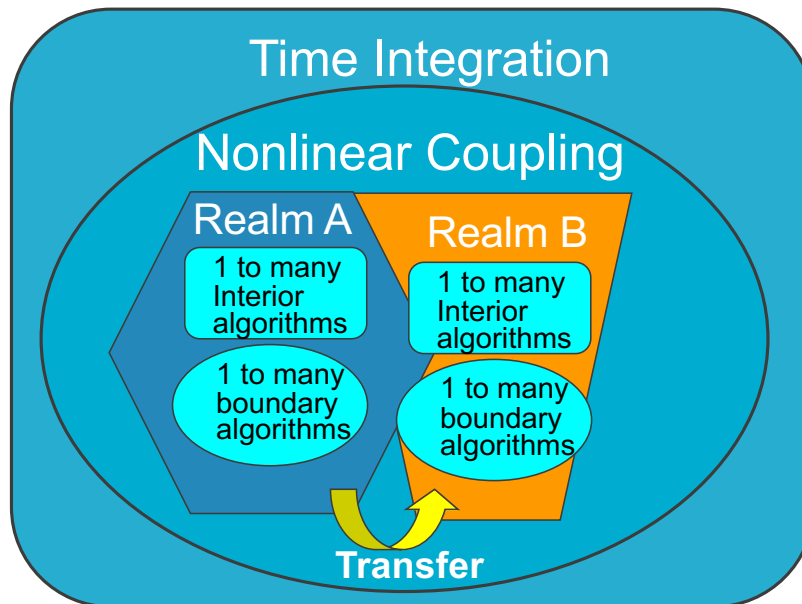


Impinging Jet DNS





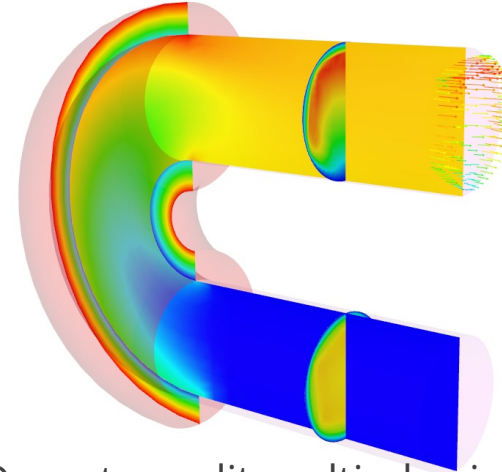
Nalu Abstractions: Polymorphic and Input File-Driven



- *Realm* specifications define the physics and desired boundary conditions
- Pre-defined *EquationSystems* (segregated or monolithic)

Operator-split multi-physics
Conjugate heat transfer coupling

- Fluids Realm
- Heat Conduction Realm



Operator-split multi-physics:

- Conjugate heat transfer coupling
 - Fluids and solid Realm



30K View: Anatomy of a Nalu Input File:YAML-based

Simulation:

linear_solvers: ← Specification of sparse Trilinos-based preconditioner/solver

transfers: ← Data transfer for multi-physics coupling

realms:

YAML enforces strict spacing and ordering

- name: realm_heatCond

boundary_conditions:

- wall_boundary_condition: bc_exposed

solution_options:

initial_conditions:

material_properties:

equation_systems:

systems:

- HeatConduction:

output:

restart:

- name: realm_fluids

TimeIntegrators:

← Time integration, e.g., BE, BDF2



<https://www.democraticunderground.com/10021540110>

Physics definitions



High-Level Elements of an Input File

systems:

- LowMachEOM:
name: myLowMach
- MixtureFraction:
name: myZ

initial_conditions:

- constant: ic_1
target_name: [block_1, ...]
value:
pressure: 0
velocity: [0.5,0.0]
mixture_fraction: 0.0

boundary_conditions:

- inflow_boundary_condition: bc_left_inflow
- wall_boundary_condition: bc_front_wall
- open_boundary_condition: bc_right_open
- symmetry_boundary_condition: bc_top
- nonconformal_boundary_condition: bc_nc

material_properties:

target_name: block_1

specifications:

- name: density
type: constant
value: 1.0
- name: viscosity
type: constant
value: 1.8e-5

material_properties:

target_name: block_1

specifications:

- name: density
type: ideal_gas
- name: viscosity
type: polynomial
coefficient_declaration:

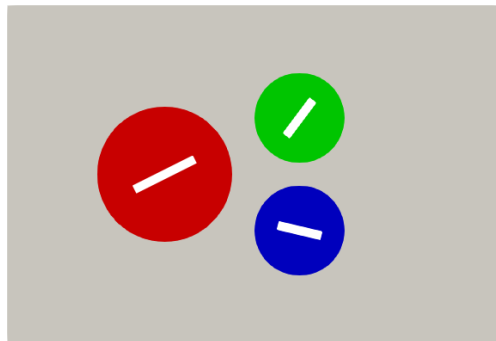
- inflow_boundary_condition: bc_left
target_name: surface_1
inflow_user_data:
velocity: [0.5,0.0,0.0]
mixture_fraction: 0.0

- wall_boundary_condition: bc_back
target_name: surface_7
wall_user_data:
user_function_name:
velocity: wind_energy
user_function_string_parameters:
velocity: [mmTop_ss7]
mixture_fraction: 1.0



A Note on Parallel Decomposition

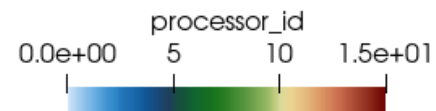
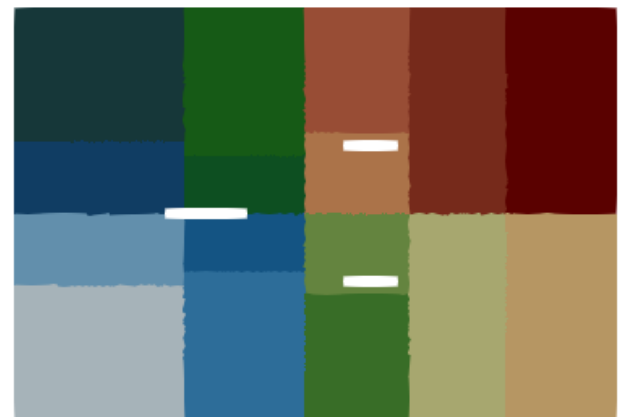
- Decomposing the mesh into small subsets and operating on these subsets in parallel provides a methodology for increased simulation time



Colored by block ID



Colored by core count (= 1) One mpi rank.



16 MPI ranks = 16x faster (hopefully)



How to Run in Parallel: Mesh Decomposition

- Given a mesh, mesh.g and myInputFile.i, if one desires to run on, e.g., 16 core case:
 1. Use pre-processing “decomposition” tools (Trilinos/install/bin)
 2. In-situ decomposition

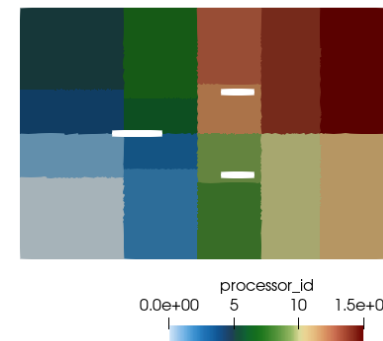


myMesh.g

2: - name: realmFluids
mesh: mesh/myMesh.g
automatic_decomposition_type: rcb

```
>/path/to/decomp -j {np} {meshName}  
>mesh.g.16.00, mesh.g.16.01, .., mesh.g.16.15
```

1: - name: realmFluids
mesh: mesh/myMesh.g
automatic_decomposition_type: rcb



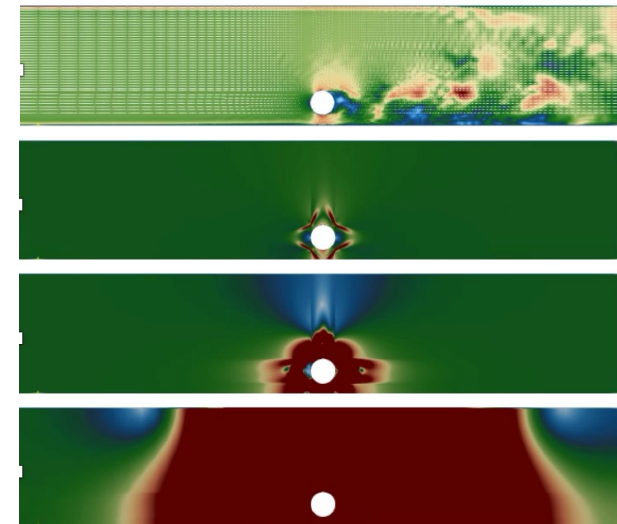
```
>mpirun --np 16 /naluParam/naluX -i input.i &
```

```
>results.e.16.00, results.e.16.01, .., results.e.16.15  
>input.log
```




A Note on Divergence

- Whether by design or poor code usage, solution results from CFD analysis for complex applications may diverge. How do I know?
- Non-finite residuals, i.e., not-a-number: "nan" (either linear or non-linear),
 - `const double norm = 0.0;`
 - `const double flux = rho*u*A/norm;`
- What if the simulation runs, however, results look very wrong? Typical causes?
 - Bad initial condition that drives nonlinear solution to diverge
 - Too large of an initial time step
 - Poor stabilization, numerical parameters, etc.
 - Poor time integration
 - Ph.D. from ICME explaining why...



EBVC flow-past 2D cylinder
Top: +NOC
Bottom se: -NOC



Test Case Input Files

- Input files are part of the Nalu regression test suite: `Nalu/reg_test/test_files`
- Mesh files are found under: `Nalu/reg_test/mesh`
- Formally, `/mesh` is a git submodule

Test Cases Highlighted:

1. `Nalu/reg_tests/test_files/dgNonConformalThreeBlade`
2. `Nalu/reg_tests/test_files/fluidsPmrChtPeriodic`

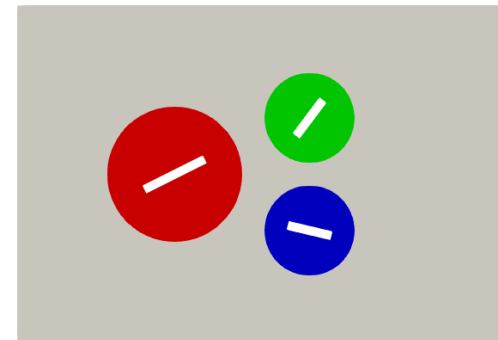
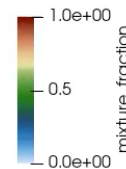
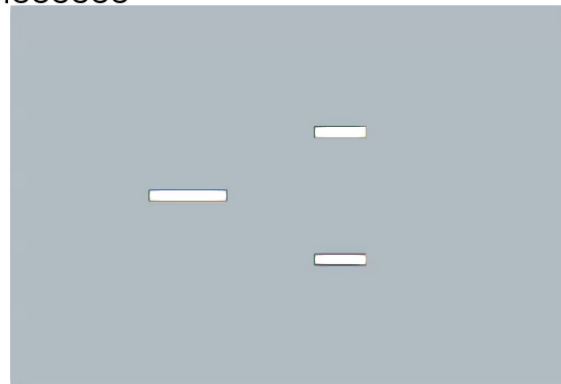
Resource: <https://nalu.readthedocs.io/en/latest/source/theory/index.html>



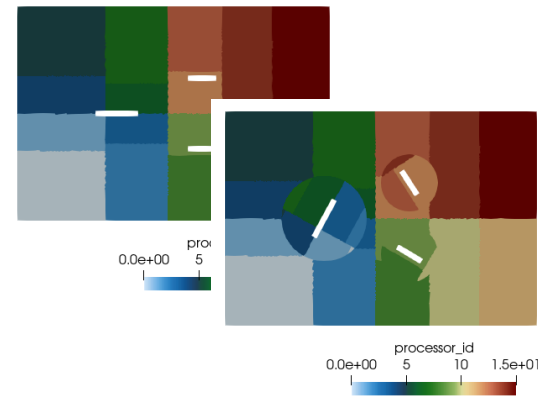
Nalu/reg_tests/test_files/dgNonConformalThreeBlade

- Physics:
 - Flow past rotating square blades ($Re = 10,000$)
- Models
 - Newtonian fluid (air) with constant properties
- Boundary Conditions
 - Inflow, open, symmetry, DG/CVFEM interface

Time: 0.000000



Domino, JCP, 2018



```
>mpirun --np 4 /naluPath/naluX -i dgNonConformalThreeBlade.i &
```



Nalu/reg_tests/test_files/dgNonConformalThreeBlade

$U\Delta t/\Delta x$

Nonlinear iterations

Equations

Review

```
Time Step Count: 43 Current Time: 0.108355
dtN: 0.002285 dtNm1: 0.00228982 gammas: 1.49947 -1.99789 0.498422
Volume 0.818029 min: 1.34303e-06 max: 7.25544e-05
Max Courant: 2.00422 Max Reynolds: 233.316 (realm_1)
Realm Nonlinear Iteration: 1/1

realm_1::advance_time_step()
NLI   Name           Linear Iter   Linear Res   NLinear Res   Scaled NLR
----
1/2   Equation System Iteration
1/1   myLowMach
      MomentumEQS      5      1.36481e-07   0.000150157   1
      ContinuityEQS    10     9.02089e-07   0.000591053   1
      PNGradPEQS       28     2.69559e-09   1.25557e-06   1
      PNGradUEQS       30     6.93157e-09   3.99347e-06   1
1/1   myZ
      MixtureFractionEQS 5     7.91662e-09   7.70262e-06   1
      PNGradZEQS       14     3.76375e-09   3.75761e-06   1
2/2   Equation System Iteration
1/1   myLowMach
      MomentumEQS      5     3.54267e-09   1.77926e-06   0.0118493
      ContinuityEQS    9     6.32285e-07   0.000379046   0.641307
      PNGradPEQS       26     2.3035e-09   1.11406e-06   0.887296
      PNGradUEQS       26     5.6359e-10   3.39699e-07   0.0850636
1/1   myZ
      MixtureFractionEQS 4     3.36865e-09   1.60783e-06   0.208738
mixFrac clipped (-) 14294 times; min: -0.0414158
mixFrac clipped (+) 2 times; max: 1.03823
      PNGradZEQS       18     1.32816e-10   6.6934e-08   0.0178129
Mass Balance Review:
Density accumulation: 0
Integrated inflow: -0.375
Integrated open: 0.3749994376540416
Total mass closure: -5.62346e-07
Mean System Norm: 6.404895358841074e-05 43 0.108355
```

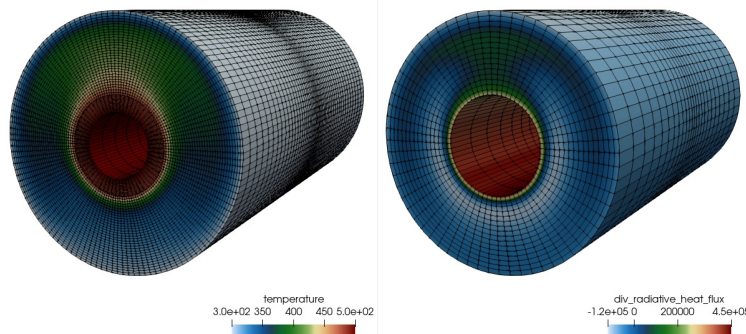
γ_i for BDF2

$\rho U L / \mu$

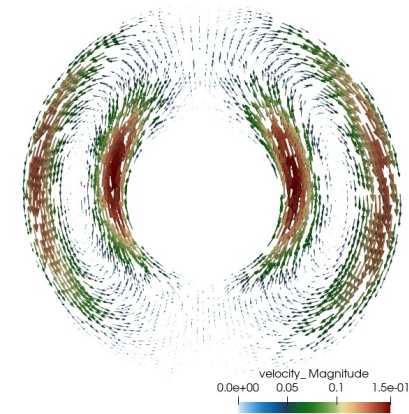


Nalu/reg_tests/test_files/fluidsPmrChtPeriodic

- Physics:
 - Uniformly emitting/absorbing participating media radiation (PMR) conjugate heat transfer (CHT) with buoyancy
- Models:
 - Newtonian fluid (air): ideal gas
- Boundary Conditions:
 - Wall, periodic



>mpirun --np 8 /naluPath/naluX -i fluidsPmrChtPeriodic.i &

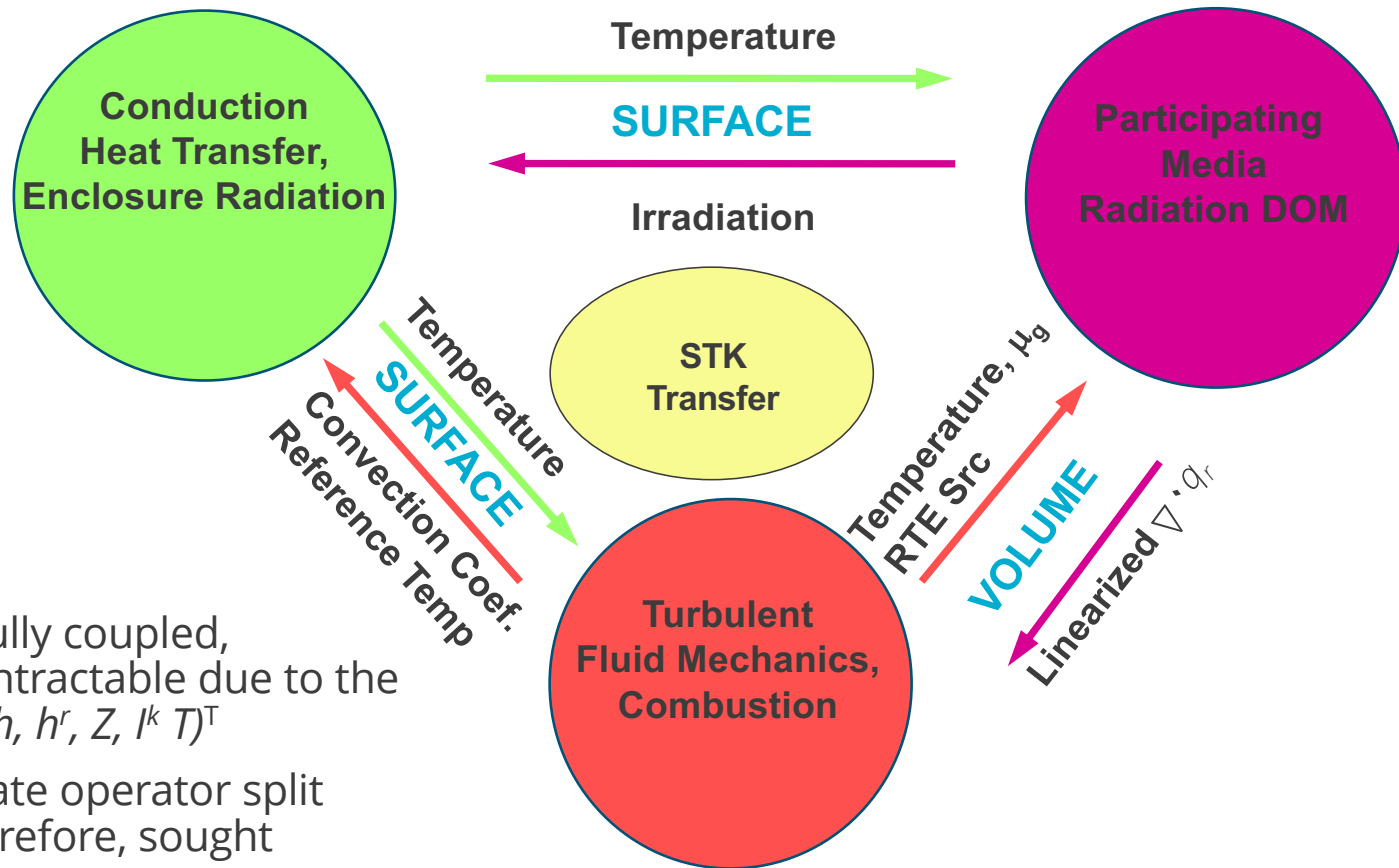


Stark#, cond/rad
 $Sk = \lambda \mu / \sigma T_i^3 \sim 0.4$

Rayleigh#, $\tau^{\text{ThermalDiff}} / \tau^{\text{Conv}}$
 $Ra = g \beta (T_i - T_o) L / Pr \alpha^2 \sim 2e6$



Nalu/reg_tests/test_files/fluidsPmrChtPeriodic



- Monolithic, i.e., fully coupled, approaches are intractable due to the size of $(u, v, w, p, h, h^r, Z, I^k T)^T$
- Stable and accurate operator split methods are, therefore, sought
- See Domino et al., AIAA, 2007



Break-out Example Using Paraview

- Live demo